

chain nodes :

19 20

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

chain bonds :

2-19 19-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 8-13 9-10 9-15 10-11  
11-12 13-14 14-15

exact/norm bonds :

2-19 7-8 7-12 8-9 8-13 9-10 9-15 10-11 11-12 13-14 14-15

exact bonds :

19-20

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 7 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom  
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 19:CLASS 20:CLASS

fragments assigned product role:

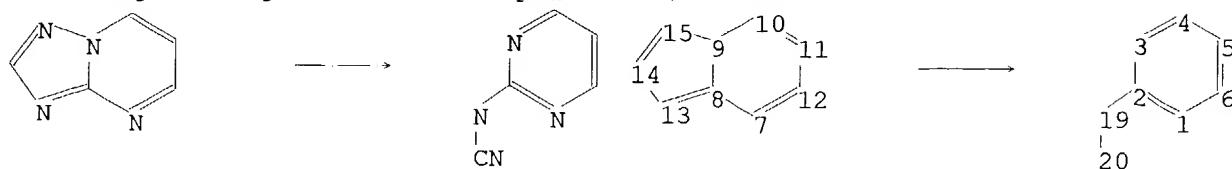
containing 1

fragments assigned reactant/reagent role:

containing 7

=&gt;

Uploading C:\Program Files\Stnexp\Queries\10615352.str



chain nodes :

19 20

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

chain bonds :

2-19 19-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 8-13 9-10 9-15 10-11 11-12 13-14  
14-15

exact/norm bonds :

2-19 7-8 7-12 8-9 8-13 9-10 9-15 10-11 11-12 13-14 14-15

exact bonds :

19-20

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 7 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 19:CLASS 20:CLASS

fragments assigned product role:

containing 1

fragments assigned reactant/reagent role:

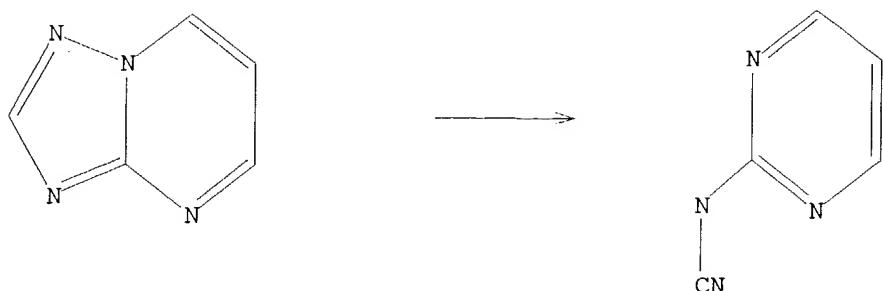
containing 7

L1 STRUCTURE UPLOADED

=&gt; d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 19:04:04 FILE 'CASREACT'  
SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS

100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 0 TO 0  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s 11 sss ful

FULL SEARCH INITIATED 19:04:12 FILE 'CASREACT'  
SCREENING COMPLETE - 19 REACTIONS TO VERIFY FROM 4 DOCUMENTS

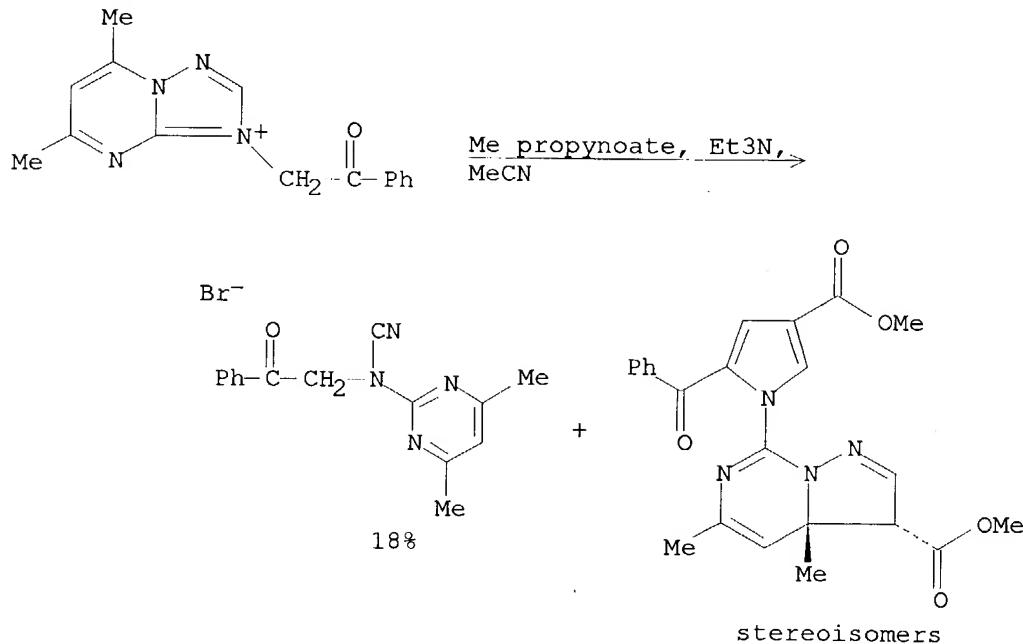
100.0% DONE 19 VERIFIED 19 HIT RXNS 4 DOCS  
SEARCH TIME: 00.00.01

L3 4 SEA SSS FUL L1 ( 19 REACTIONS)

=> d 13 1-4 bib,ab,crdref

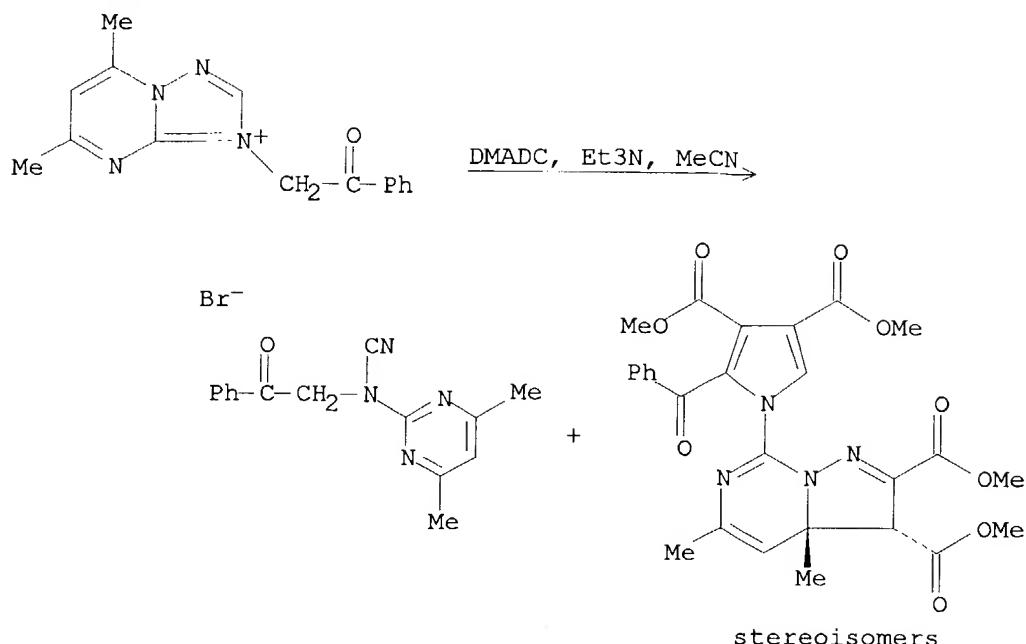
L3 ANSWER 1 OF 4 CASREACT COPYRIGHT 2004 ACS on STN  
 AN 108:186688 CASREACT  
 TI An unexpected double cycloaddition of [1,2,4]triazolo[1,5-a]pyrimidine N-ylide with activated acetylenes and alkenes  
 AU Hori, Mikio; Kataoka, Tadashi; Shimizu, Hiroshi; Imai, Eiji; Tanaka, Kiyomi; Kimura, Kazuhiko; Hashimoto, Yoshinobu; Inagaki, Satoshi; Goto, Naomi; Kido, Masaru  
 CS Gifu Pharm. Univ., Gifu, 502, Japan  
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (11), 2531-7  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DT Journal  
 LA English  
 AB The reaction of 5,7-dimethyl-[1,2,4]triazolo[1,5-a]pyrimidinio-3-phenacylide I (R = Ph, 4-BrC<sub>6</sub>H<sub>4</sub>) with activated acetylenes, R<sub>1</sub>C.tplbond.CCO<sub>2</sub>Me (R<sub>1</sub> = H, CO<sub>2</sub>Me), gave 1:2 adducts. The structures of the products were determined as 3,3a-dihydropyrazolo[1,5-c]pyrimidine derivs. II by hydrolysis, <sup>1</sup>H and <sup>13</sup>C NMR, and X-ray crystallog. MO calcns. of model compds. suggested that an intermediate 1:1 adduct would be less reactive than I. However, despite many attempts, isolation of the 1:1 adduct was unsuccessful. Formation of the 1:2 adducts is explained by an equilibrium between 1:1 adduct III and the starting materials.

RX(2) OF 13



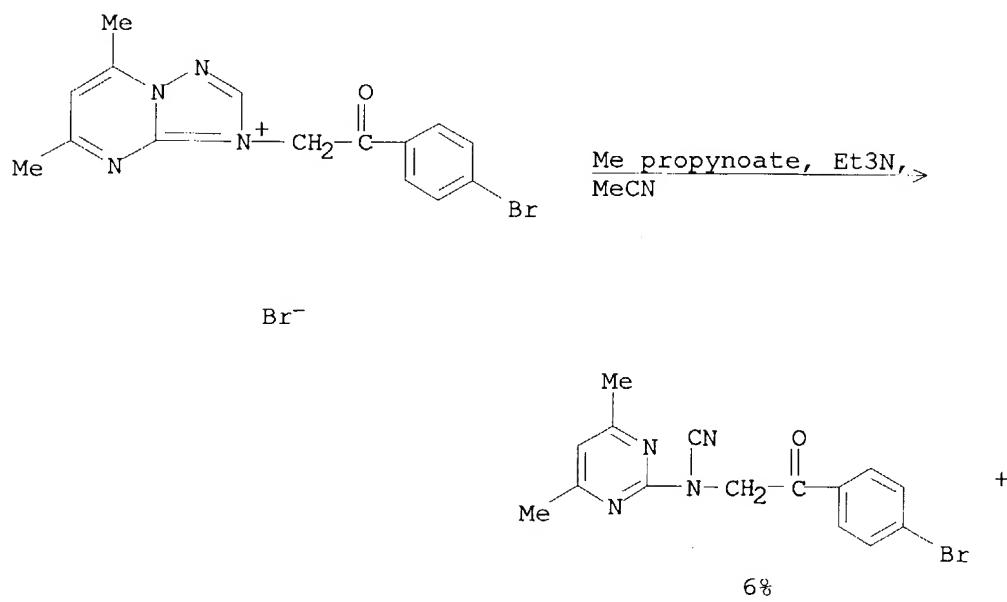
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2531-7, 1987

RX(3) OF 13

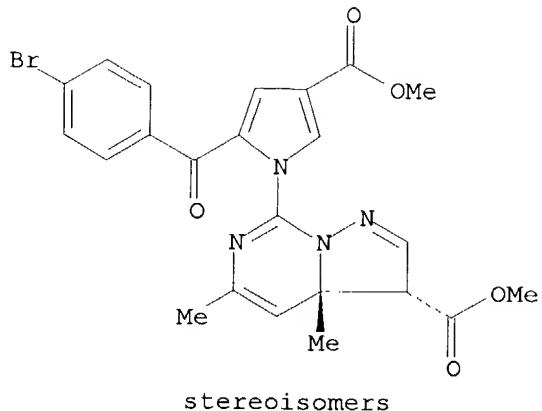


REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2531-7; 1987

RX(4) OF 13

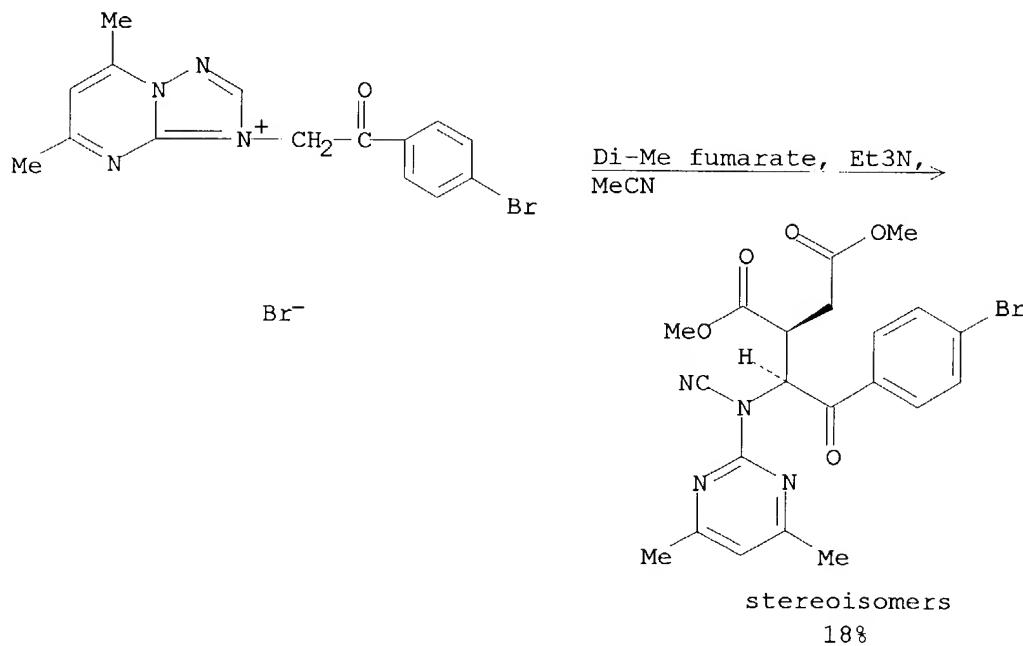


RX(4) OF 13



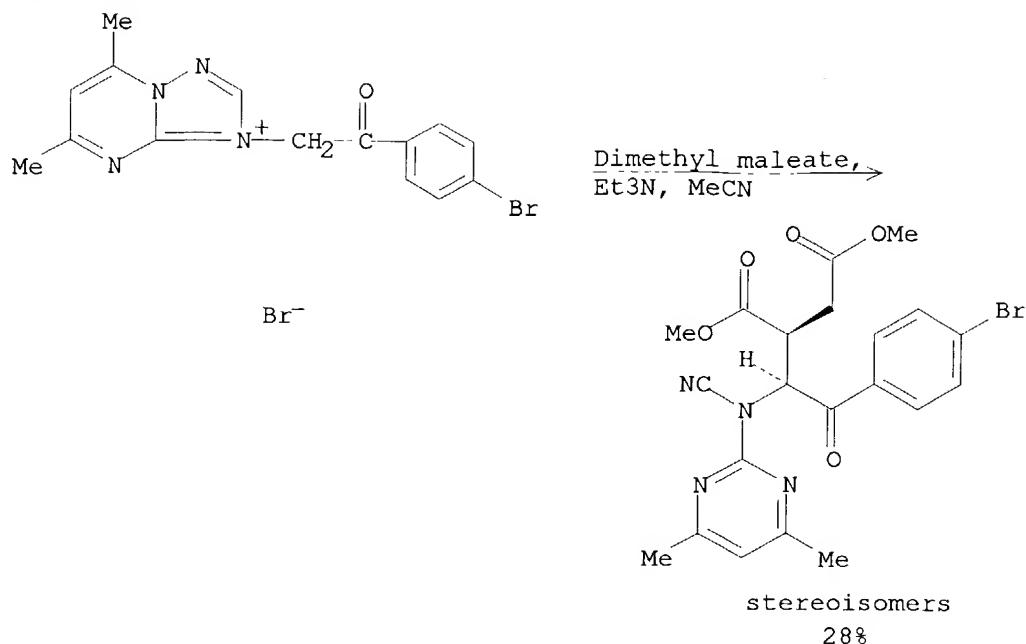
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2531-7; 1987

RX(9) OF 13



REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2531-7; 1987

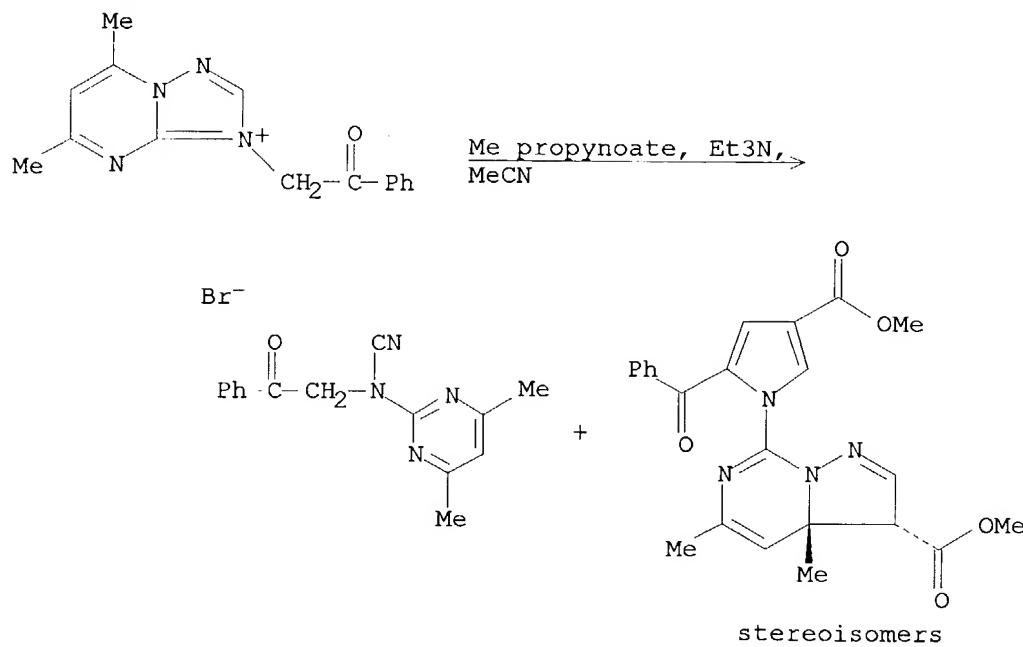
RX(10) OF 13



REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2531-7; 1987

L3 ANSWER 2 OF 4 CASREACT COPYRIGHT 2004 ACS on STN  
 AN 106:18477 CASREACT  
 TI Ylidé-induced ylide formation. A novel double cycloaddition reaction of a [1,2,4]triazolo[1,5-a]pyrimidinium ylides  
 AU Hori, Mikio; Kataoka, Tadashi; Shimizu, Hiroshi; Imai, Eiji; Tanaka, Kiyomi; Kimura, Kazuhiko; Hashimoto, Yoshinobu; Kido, Masaru  
 CS Gifu Pharm. Univ., Gifu, 502, Japan  
 SO Tetrahedron Letters (1986), 27(6), 717-18  
 CODEN: TELEAY; ISSN: 0040-4039  
 DT Journal  
 LA English  
 AB Treatment of 5,7-dimethyl-3-phenacyl 1,2,4-triazolo[1,5-a]pyrimidinium ylide with Me propionate leads to a novel double cycloaddn. to give the 3,9-dihydropyrazolo[1,5-c]pyrimidine I.

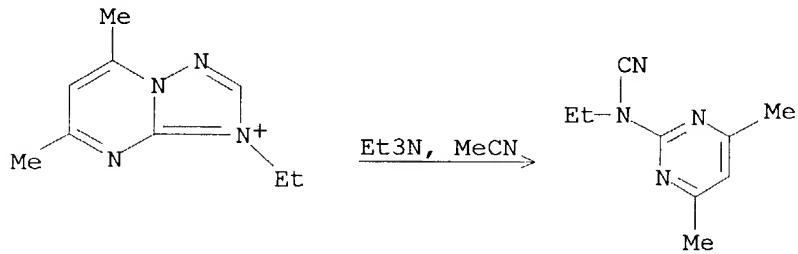
RX(1) OF 1



REF: Tetrahedron Letters, 27(6), 717-18; 1986

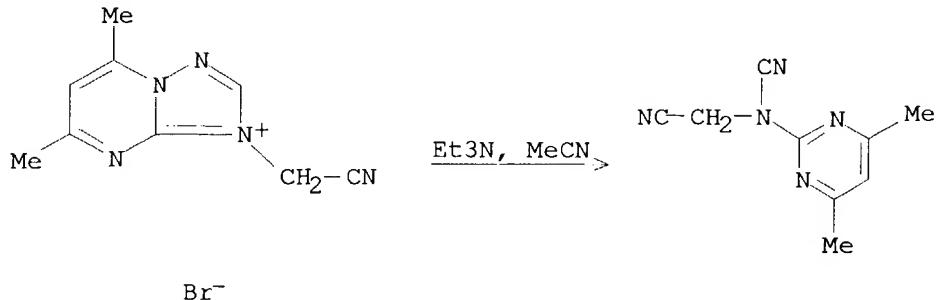
L3 ANSWER 3 OF 4 CASREACT COPYRIGHT 2004 ACS on STN  
 AN 105:153023 CASREACT  
 TI Generation of [1,2,4]triazolo[1,5-a]pyrimidine N-ylides and their ring transformation reactions  
 AU Hori, Mikio; Tanaka, Kiyomi; Kataoka, Tadashi; Shimizu, Hiroshi; Imai, Eiji; Kimura, Kazuhiko; Hashimoto, Yoshinobu  
 CS Gifu Pharm. Univ., Gifu, 502, Japan  
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (11), 2333-6  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DT Journal  
 LA English  
 AB Triazolopyrimidine was quaternized with RCH<sub>2</sub>Br or RCH<sub>2</sub>I (R = Me, cyano, CO<sub>2</sub>Me, Bz, COC<sub>6</sub>H<sub>4</sub>Br-4) in refluxing acetone to yield salts I. Treatment of I with Et<sub>3</sub>N produced cyanamidopyrimidines II. I(R = Bz), when treated with Et<sub>3</sub>N gave 2-(2-imino-5-phenyl-2,3-dihydrooxazol-3-yl)pyrimidine in 64.4% yield. The latter on treatment with R<sub>1</sub>OH (R<sub>1</sub> = Me, Et, CHMe<sub>2</sub>), Et<sub>2</sub>NH, or H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OH under acidic conditions afforded the ring transposition products imidazolypyrimidines III (R<sub>2</sub> = R<sub>1</sub>O, Et<sub>2</sub>N, HOCH<sub>2</sub>CH<sub>2</sub>NH). The reaction mechanism for the novel thermolysis of I is discussed.

## RX (6) OF 36



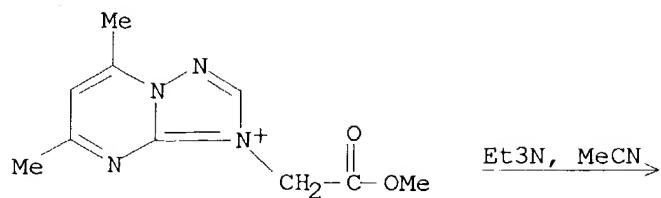
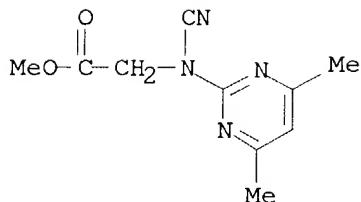
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

## RX (7) OF 36



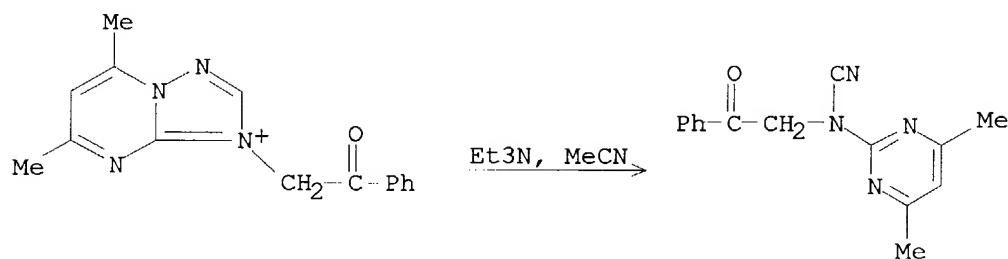
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

## RX (8) OF 36

 $\text{Br}^-$ 

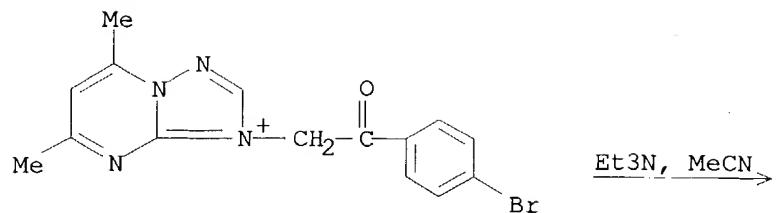
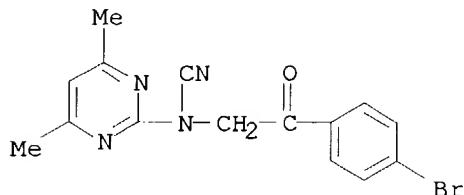
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

## RX (9) OF 36

 $\text{Br}^-$ 

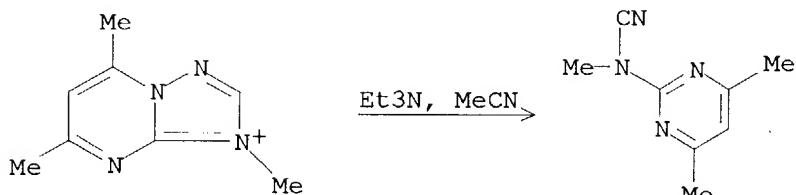
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

## RX(10) OF 36

 $\text{Br}^-$ 

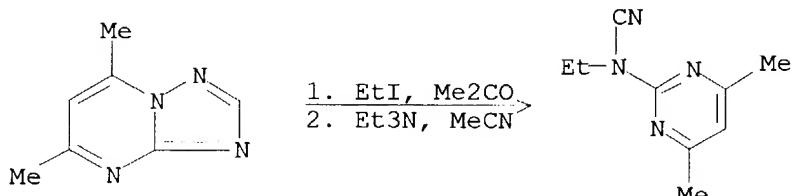
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

## RX(11) OF 36



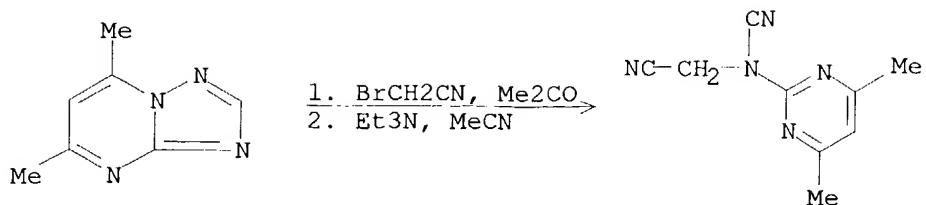
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

## RX(19) OF 36 - 2 STEPS



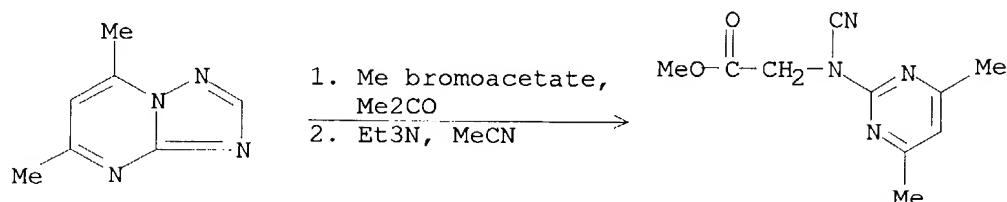
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

## RX(20) OF 36 - 2 STEPS



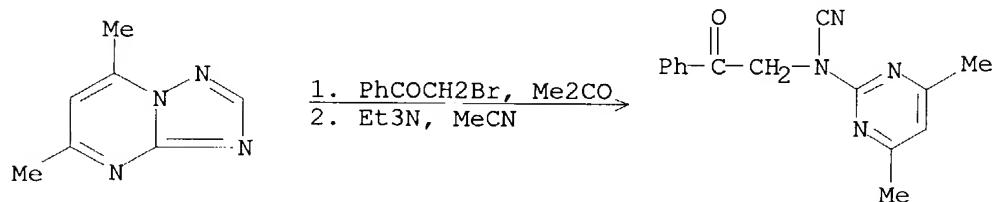
REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

## RX(21) OF 36 - 2 STEPS



REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

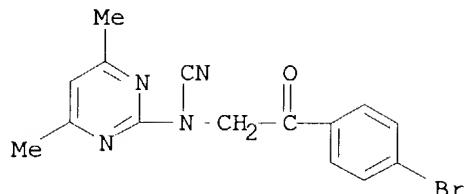
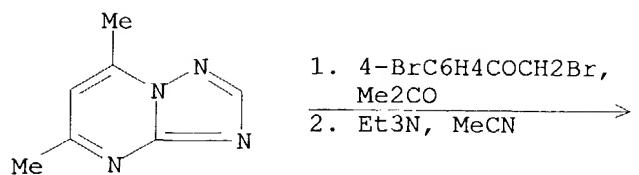
## RX(22) OF 36 - 2 STEPS



REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

NOTE: 1) One mole of base

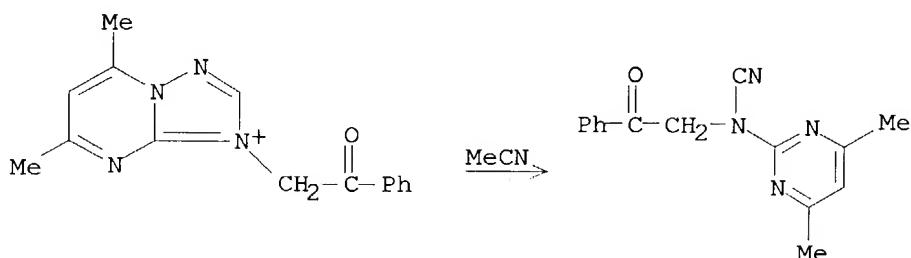
RX(24) OF 36 - 2 STEPS



REF: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), (11), 2333-6; 1985

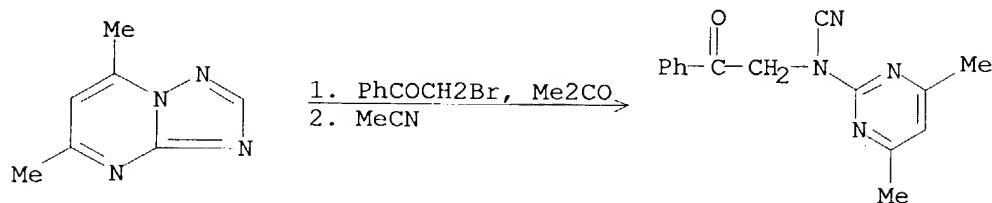
L3 ANSWER 4 OF 4 CASREACT COPYRIGHT 2004 ACS on STN  
 AN 103:87834 CASREACT  
 TI Thermolysis of [1,2,4]triazolo[1,5-a]pyrimidine N-ylides  
 AU Hori, Mikio; Tanaka, Kiyomi; Kataoka, Tadashi; Shimizu, Hiroshi; Imai, Eiji; Kimura, Kazuhiko; Hashimoto, Yoshinobu  
 CS Gifu Pharm. Univ., Gifu, 502, Japan  
 SO Tetrahedron Letters (1985), 26(10), 1321-2  
 CODEN: TELEAY; ISSN: 0040-4039  
 DT Journal  
 LA English  
 AB Unstable 5,7-Dimethyl[1,2,4]triazolo[1,5-a.]pyrimidinio-3-phenacylide I generated by treating the iminium salt II with 1 equivalent of Et<sub>3</sub>N under went a thermal ring cleavage to give the pyrimidine III. However, II reacted with 2 equivs. of Et<sub>3</sub>N to afford the 2-iminooxazoline IV reacted with alcs and amines to give imidazoles.

## RX(2) OF 26

 $\text{Br}^-$ 

REF: Tetrahedron Letters, 26(10), 1321-2; 1985  
 NOTE: 1 equiv. of triethylamine

## RX(8) OF 26 - 2 STEPS



REF: Tetrahedron Letters, 26(10), 1321-2; 1985  
 NOTE: 2) 1 equiv. of triethylamine

10/615,352

=> log y			
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION	
FULL ESTIMATED COST	124.30	124.51	
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CA SUBSCRIBER PRICE	-2.64	-2.64	

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